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Determination of the contact angle from transversality conditions of the Lagrange variation problem of wetting

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In recent years, there has been an increase in studies focused on the size-dependent contact angle. In the case of the sessile axial symmetric droplet, the size dependence often is explained by the contribution of the line tension to the Helmholtz free energy as a consequence, the modified Young's equation. There are two major points of view on the contribution mechanism. According to the first point of view, the liner tension is a function of the contact angle; according to another one, the line tension is a function of the three-phase contact line torsion and geodesic curvature. However, in the case of the straight contact line, it is impossible to determine the influence of the line tension of the three-phase contact line on the contact angle.
We propose a model of the line tension of the three-phase contact line influence on the contact angle. We consider the line tension as a thermodynamic work on the deformation transition region on the three-phase border to determine the influence. Therefore, the line tension becomes a function of the dividing surface curvature on the contact line. Then, the Helmholtz free energy of a unit of the cylindric nanodroplet length Δx with the additional condition of incompressibility of the nanodroplet liquid is:

$$F\left[z\left(y\right)\right]=\int\limits_{x}^{x+\Delta x}dx\int\limits_{-r}^{r}dyL\left(y,z,z',z''\right)=$$

$$\int\limits_{x}^{x+\Delta x}dx\int\limits_{-r}^{r}dy\left\{\gamma_{sv}-\gamma_{sl}+\gamma_{lv}\left[\frac{z''^2}{\left(1+z'^2\right)^{3/2}}\right]\sqrt{1+z'^2}+\frac{1}{r}\tau\left[\frac{z''^2}{\left(1+z'^2\right)^{3/2}}\right]+\lambda yz'\right\}, \quad (1)$$

where, *2r* – the width of the nanodroplet base, γ – the surface tension between liquid/vapor, solid/liquid and solid/vapor, τ – the line tension of three-phase contact line, λ – Lagrange multiplier. The transversality conditions of the Lagrange problem with moving boundary for the functional containing the second-order derivative are:

$$\left[L-z'\left(\frac{\partial L}{\partial z'}-\frac{d}{dy}\frac{\partial L}{\partial z''}\right)+\left(\frac{z'\arctan\left(z'\right)\left(1+z'^2\right)-z'^2}{y\left(\arctan\left(z'\right)-z'\right)}-z''\right)\frac{\partial L}{\partial z''}\right]_{y=-r,r}=0. \quad (2)$$

The contact angle can be obtained by minimization of the Helmholtz free energy functional with the application of the transversality conditions:

$$\left(1-\left(\frac{\delta_c}{R}\right)+o\left(\frac{\delta_c}{R}\right)^2\right)\cos\left(\theta\right)=\frac{\gamma_{sv}-\gamma_{sl}}{\gamma^{\infty}{}_{lv}}-\frac{\tau}{\gamma^{\infty}{}_{lv}R\sin\left(\theta\right)}, \quad (3)$$

where, δ_c – the Tolman length, θ – the contact angle, $\gamma^{\infty}{}_{lv}$ – the surface tension of a flat surface, R – the radius of the liquid-vapor interface curvature.
It has been shown that the contact angle depends on the line tension of the straight three-phase contact line.

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